

# Adsorption of Helium Atoms on Two-Dimensional Substrates

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## Abstract

© 2016, Springer Science+Business Media New York. The study of the adsorption phenomenon of helium began many decades ago with the discovery of graphite as a homogeneous substrate for the investigation of physically adsorbed monolayer films. In particular, helium monoatomic layers on graphite were found to exhibit a very rich phase diagram. In the present work we have investigated the adsorption phenomenon of helium atoms on graphene and silicene substrates by means of density functional theory with Born-Oppenheimer approximation. Helium-substrate and helium-helium interactions were considered from first principles. Vibrational properties of adsorbed monolayers have been used to explore the stability of the system. This approach reproduces results describing the stability of a helium monolayer on graphene calculated by quantum Monte Carlo (QMC) simulations for low and high coverage cases. However, for the moderate coverage value there is a discrepancy with QMC results due to the lack of helium zero point motion.

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## Keywords

Adsorption, Density functional theory, Graphene, Helium, Silicene